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MATERIAL SELECTION GUIDE DERIVED FROM MATERIAL - CHEMICAL COMPATIBILITY DATABASE: FEASIBILITY BASED ON DATABASE AND PREDICTIVE MODEL EVALUATION

Wendel J. Shuely

RESEARCH DIRECTORATE

James J. McNeely

CHEMICAL/BIOLOGICAL INFORMATION AND ANALYSIS CENTER
Edgewood, MD 21040

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Shuely, Wendel J. (CRDEC), and McNeely, James J. (CBIAC)

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The identification and selection of materials survivable in an NBC environment is an important consideration throughout the Department of Defense. The U.S. Army Chemical Research, Development and Engineering Center was asked by other services to evaluate the feasibility of compiling a list of materials that are survivable in a CB environment and compatible with current decontamination substances. The feasible characteristics of a candidate NBCCS Materials Guide are discussed herein. Thermodynamic predictive methodologies evaluated in the studies included approaches on polymer solubility phase diagrams, equation-of-state, and universal group contribution activity coefficient estimates. The studies required to generate the guide and the resources required are estimated. The evaluation concluded that a limited but potentially useful NBCCS Materials Guide appears to be feasible.

14. SUBJECT TERMS

NBCCS	Material compatibility
Chemical defense	Polymer-liquid interaction
Material(s) database	Chemical defense materials database

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PREFACE

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The CRDEC has established the MSSD within the Advanced Systems Concepts Directorate to assist project managers throughout the Department of Defense with their NBCCS responsibilities.

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FROM MATERIAL - CHEMICAL COMPATIBILITY DATABASE:
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1. INTRODUCTION

The identification and selection of survivable materials in an NBC environment is an important consideration throughout the Department of Defense (DoD). About one fourth of the queries by the Chemical Biological Information and Analysis Center (CBIAC), Aberdeen Proving Ground, MD, concern materials, and about one-half of the CBIAC resources are expended in an attempt to respond to chemical defense (CD) material questions.

This study was initiated as a response to a Joint Panel request on CB Defense. The U.S. Army Chemical Research, Development and Engineering Center (CRDEC) has informally accepted the long-term task of compiling a materials guide on survivable materials in a CB environment that are compatible with current decontamination substances.

A systematic evaluation of the status and future capabilities of a chemical materials database requires consideration of the following three elements: liquids, material compositions, and test properties. Liquids were evaluated based on deriving a logical database search strategy that corresponded to the actual material selection criteria implied by the NBCCS regulation. In addition, we consider the obsolescence of the database contents due to evolution of decontamination solution contents or the changes in a threat contaminant with time.

Materials were evaluated with respect to the fraction of materials represented in the database relative to the universe of either all generic materials or all individual materials. The advantages and risks of equating a specific composition to a generic composition are discussed.

Test and property database content was evaluated based on the complexity of identifying material properties that predict component performance. Because this is a classical and rather common-place problem area in material science, the actual difficulty involves the need to emphasize to design engineers that different sets of material properties and tests are required for each unique type of performance (e.g., optical, electronic, mechanical, etc.).

The Chemical Defense Materials Database (CDMD) is presently a single, query-based system. Data retrieval is based on a one-at-a-time liquid/test property/material matrix. The CDMD does not have a comprehensive "self-inventory" facility that would report the presence or absence of data for broad categories of test properties, materials, and/or liquids to the manager or user. The initial overviews of the CDMD's contents are documented here. Otherwise, these overviews were obtained by a sequence of an ad hoc inventories of the CDMD that revealed the contents in selected layers of detail. These partial inventories were necessary and critical to evaluating

the feasibility of generating a materials guide and planning the direction of ongoing database research and development.

The feasible characteristics of a candidate NBCCS Materials Guide are discussed herein, the studies required to generate the guide are described, and the resources required are estimated.

2. RESTRICTIONS ON DEVELOPING AN NBCCS MATERIALS GUIDE

2.1 Rationale.

There are two extremes concerning the feasibility of developing a NBCCS Materials Guide.

The most optimistic extreme would envision a listing that corresponds to a Qualified Product List (QPL). Selection and use of a material from a hypothetical NBCCS material QPL would meet all NBCCS responsibilities. The complexity of vulnerability and criticality issues does not allow the simplistic QPL-type approach.

The other extreme suggests the materials selection issues are so complex that only a repeat of system developmental testing, military specification, or RAM testing of a "before" versus an "after" NBC scenario is useful for material selection.

In between these extremes lies the usual development process in which standard material tests (e.g., American Society for Testing and Materials (ASTM), Military Standards, etc.) are employed to identify and select material compositions for applications. These material tests are correlated to material end-use performance. A parallel strategy can be applied to provide "before" versus "after" property degradation results for a set of agent contaminants and decontaminants. The evaluation of a large database of this type could also generate a list of candidate materials that might be NBCCS survivable for all agents/decontaminants. Several examples can be provided that demonstrate some difficulties that must be dealt with to provide this list, which is due to either the inherent complexities or to the limitations of the current database.

2.2 Identical Material Composition with Different Performance Criterion.

An inherent limitation is that each material application has a different performance criterion. There are several independent types of material properties (Table 1). A significant degradation in mechanical tensile properties may not be critical to a specific optical, electrical, or thermal application. However, there is no way an NBCCS Materials Guide can "recognize" the enormous variety of complex performance requirements throughout DoD systems.

Table 1. Material Property Classes

Mechanical	Electrical
Optical	Thermal

2.3 Concurrent Resistance to Several Liquids.

Another inherent complexity in material selection is that the material must not have relevant critical properties degraded by any of an entire set of liquids (i.e., the set includes all of the threat liquids and/or all of the current decontamination solutions that might be used on that surface). Therefore, a material cannot be placed on a candidate NBCCS Materials Guide if any one of several liquids causes performance degradation.

In addition, two criteria relevant to materials selection are ability of agents to be decontaminated and hardness for decontaminants (sometimes, agents). This means that the set of each of the agent decontaminability test properties must be logically compared with the sets of decontaminant (and/or an agent) hardness properties to find common elements (Figure 1). The resultant material list could be quite short. A systematic, one-by-one relaxation of property degradation levels would cause the permutation of many hierarchies of material rankings. For example, for ratings of only negligible (N) and moderate (M):

N, N, N, N, N

M N N N N

M M N N N

...Etc.

2.4 Evaluation of Decontamination Solution Content with Time.

Another inherent limitation is the evolution and change of decontamination solution composition over time (Figure 2). The codes for the decontamination solutions are in Table 2. When additional or replacement [DS3(PGMME), DAM] decontamination solutions are fielded, new test data must be generated, searches evaluated, and new candidate materials lists generated. Generally, new decontamination solutions have a high priority requirement to be compatible with a higher fraction of materials. However, the new decontamination solution might degrade a smaller but different set of material types.

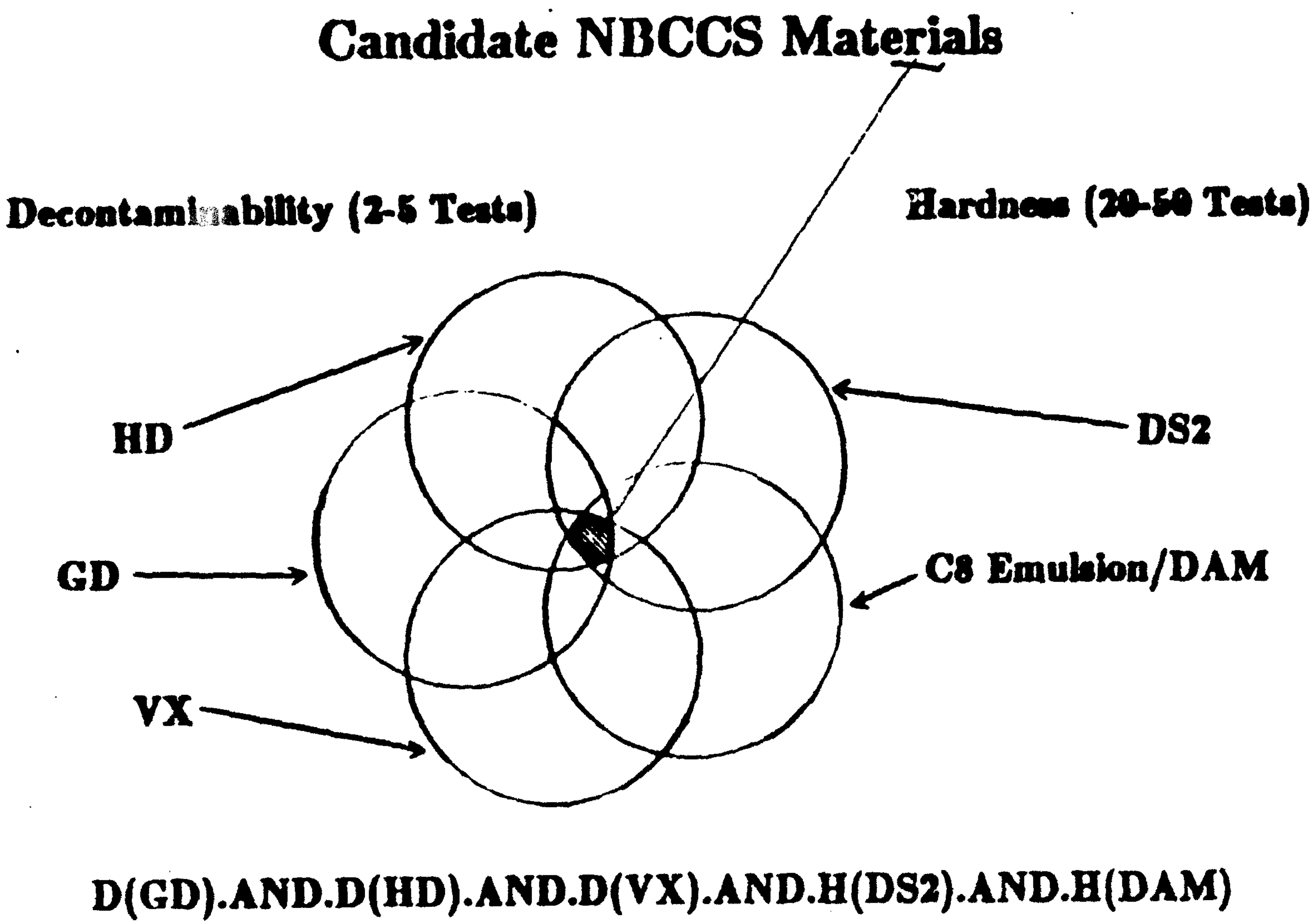

Figure 1. Diagrammatic Representation of NBCCS Material Requirement for Contaminant Decontaminability and Decontaminant Hardness by Logical "AND" Operator

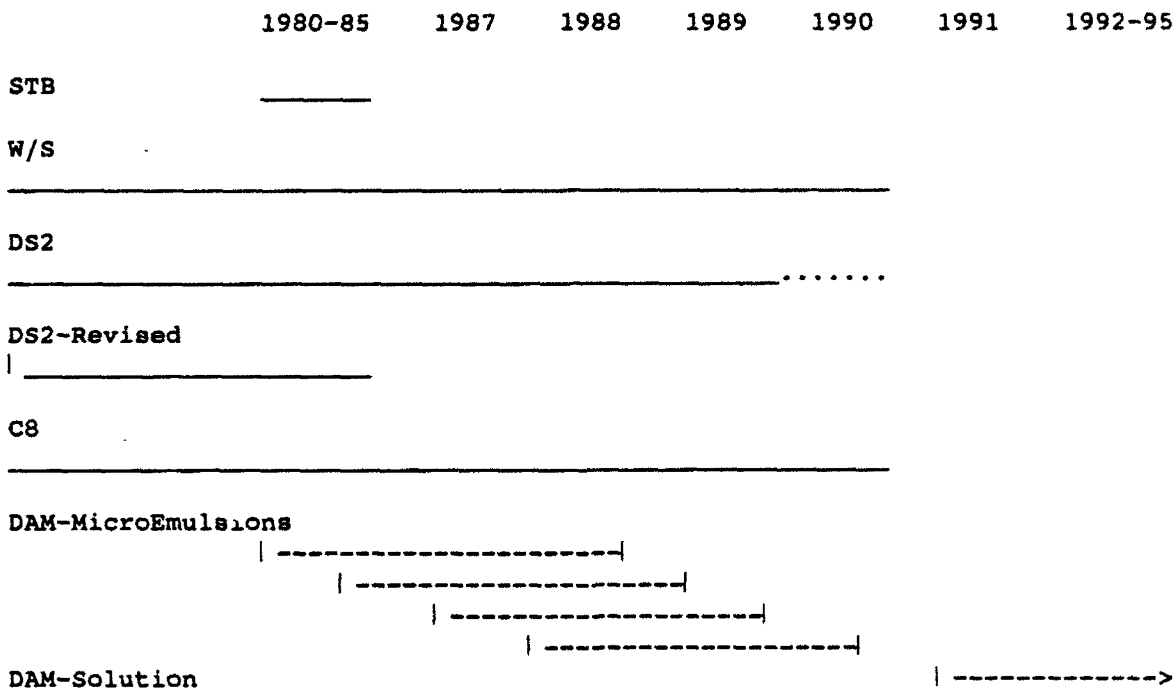

Figure 2. Decontamination Solutions: Fielded and Developmental Solutions Versus Time Interval

Table 2. Decontamination Solution Code Names

DAM:	Decontaminating Agent, Multipurpose
C8:	Fielded German Decontamination Microemulsion
STB:	Super Tropical Bleach: Terrain Decontamination Powder
DS2:	Decontamination Solution for Equipment
W/S:	Surfactant in Water

2.5 Influence of Partially Filled Database.

The above complexities (Sections 2.2, 2.3, and 2.4) presume that the data is available in each material liquid property element of the database to perform a logical comparison. The contents of the CDMD[1,2] are somewhat randomly filled (Table 3); therefore, systematic "search and identify" strategies fail. One can see that a missing datum (Table 3) prevents a systematic comparison, even though half the elements are filled. It is doubtful whether any complete liquid-property data set exists for any material in the CDMD (as of 1991). This includes relaxing and broadening the search from a specific material composition to allow including different material compositions in a general generic class.

Table 3. Simplified Listing of Chemical Defense Material Database Contents

Material (M) Test Property (T)		Liquid (L) L1	L6
M1:	T1	nd	123. Negligible
	T60	456. Moderate	nd
M11,000:	T1	78. Negligible	nd
	T60	nd*	910. Severe

*nd = not determined

2.6 Estimates of the Magnitude of a Materials Database.

A useful exercise would be to assume certain strategies for completely filling a hypothetical future CDMD based on a material x properties x liquid product and then calculating the current percentage completed for each size of a hypothetically filled CDMD (Tables 4 and 5).

Table 4. Polymeric Materials: Number of Generic Classes and Specific Commercial Formulations

	PLASPEC[3] Generic/Commercial Type/Formulations
Plastics + Elastomers	65/11,500
Plastics	57/10,700
Thermoplastics	46/9,700
Thermosets	11/1,000
Elastomers	8/800

Table 5. Estimate of the Percent of CDMD Elements Entered (One Material/Liquid/Test) Versus Various Strategies for a Completed Database

Strategy	Number of Materials	Properties	Liquids	Percent
Current CDMD	655	60	6	1
All Materials	11,000	60	6	.07
1 each Generic	150	60	6	5
Screened Resistant Materials	180 (3 x 60)	60	6	5
Screened Resistant Materials	30 (3 x 10)	10	6	60
Non-resistant Irreplaceable	Unknown	60	6	Unknown
Fielded	Unknown	60	6	Unknown

Given the current 655 materials, 60 properties, and assuming only 6 liquids (3 agents, 2-3 decontaminants), only 1% of the current CDMD is complete.

As an upper bound, including all commercial materials (11,000) would yield a 0.07% complete database.

A strategy of including only one of each generic material class shows that this limited dataset is 20 times (100/5%) the current database.

A strategy of identifying and measuring only these screened materials with good resistance for each property would also require a database about 20 times the current contents.

An analogous, but riskier, strategy of reducing the number of properties to 10 orthogonal properties would require only doubling the current CDMD contents, which begins to appear feasible.

These strategies are concerned with material selection for future systems. Other strategies might be concerned with nonreplaceable, nonsurvivable materials that must be fielded; some material database characterizations of these might be useful and would place more demands on database expansion. Evaluation of materials in fielded systems is another requirement placed on the CDMD with unknown content and matrix size.

2.7 Inventory of the Frequency of Test and Property Data.

An inventory of the occurrence of property data types within the CDMD can be provided (Table 6). The (rounded) number of tests are listed with percent of total in parentheses. Five test properties account for 70% of the total, and 30% are distributed over the other 55 test properties. Four of the five are relevant to specific types of hardness, and two are relevant to decontaminability.

Table 6. Inventory of Occurrence of Property Data for a Single Material Liquid Pair (1991) with Relevance to Decontaminability or Hardness

	Property	Number	Relevance Code
1st	Weight Change (dimensions)	600 (22%)	D
2nd	Tensile Properties	600 (22%)	H
3rd	Corrosion Rate	300 (12%)	H
4th	Cumulative Permeation	200 (7%)	D,H
5th	Hardness, Shore	200 (7%)	H
55	Other Properties 1-50 each	800 (30%)	H

D = Decontamination
H = Hardness

3. PROGRAM FOR PROVIDING CANDIDATE NBCCS MATERIALS GUIDE

3.1 Scope.

There are three interrelated tasks that should be pursued concurrently to provide a Candidate Materials Guide to be used in ranking and recommending materials for NBCCS:

- Exploit existing commercial databases that numerically rank and classify the degree of liquid material interaction

- Exploit existing commercial compatibility compilations (numerous) and databases (few)

- Accelerate the systematic evaluation of the CDMD to provide interim and updated listings of candidate NBCCS materials

3.2 Polymer Liquid Interaction Rankings.

The liquid material interaction rankings are derived from commercial databases that employ properties of liquid and polymeric materials. The properties of any unique liquid (e.g., chemical contaminants and decontaminants) must first be determined.[4]

Relative rankings, ranging from highly resistant to nonresistant, are listed using HD as an example (Table 7). Table 7 lists the polymeric material name, the vector value showing the relative ranking, and the results of solubility test ASTM D3132 to check and validate the database rankings. Higher values of the ranking vector denote the more resistant materials for the liquid HD. Available ASTM D3132 results are listed and confirm the rankings. Teflon, tedlar, and butyl rubber are correctly ranked as resistant to HD, and this ranking is confirmed by the Insoluble (I) ASTM D3132 test result. An example of computer output for other materials is provided in Table 8.

Table 7. Hansen Cohesion Parameter Rankings/Predictions of Polymers Liquid Interaction: HD

Polymer	Vector	Experiment ASTM D3132
Poly(vinylidenefluoride): Tedlar	2.02	I est
Nylon: Versamid 930	1.50	nd
Polyethylene, Chlorosulfonated: Hypalon 20	1.42	nd
Polytetrafluoroethylene: Teflon	1.26	I
Polyvinylchloride: Vipla KR	1.18	I
Polyisoprene: Cariflex IR305	1.18	I
Aromatic Hydrocarbon Resin: Piccopale 110	1.18	nd
Aromatic Hydrocarbon Resin: Piccolyte S100	1.13	nd
Isobutylene: Butyl Rubber	1.02	I

nd = not determined
I = Insoluble
I est = Insoluble, estimate

Table 8. Example of Computer Printout of Polymer Liquid Interaction Rankings for 120 Polymeric Materials[4].

Polymers						
				DP	PP	HP
Name:	Bis(2-chloroethyl) Sulfide			19.40	7.80	5.00
Red	No.	Polymer	DP	PP	HP	R
0.706	1	CELLIT BP-300	16.60	12.00	6.70	10.20
1.052	2	CELLIDORA A	18.20	12.40	10.80	7.40
0.803	3	ETHOCEL HE10	17.90	4.30	3.90	5.90
0.191	4	ETHOCEL STD20	20.10	6.90	5.90	9.90
0.852	5	ARALD DY025	14.00	7.40	9.40	13.70
0.490	6	EPIKOTE 828	23.10	14.60	5.00	20.50
0.581	7	1001	20.00	10.32	10.11	10.02
0.793	8	1004	17.40	10.50	9.00	7.90
0.818	9	1007	21.00	11.10	13.40	11.70
0.745	10	1009	19.30	9.37	10.95	8.26
0.850	11	PKHH	23.40	7.20	14.80	14.90
0.898	12	VERSAMID 100	23.80	5.30	16.20	16.10
0.974	13	VERSAMID 115	20.30	6.60	14.10	9.60
0.896	14	VERSAMID 125	24.90	3.10	18.70	20.30
0.870	15	VERSAMID 140	26.90	2.40	18.50	24.00
0.835	16	DESMOPHEN 651	17.70	10.60	11.60	9.50
0.827	17	DES 800	19.10	12.20	9.90	8.00
0.659	18	DES 850	21.54	14.94	12.28	16.78
0.841	19	DES 1100	16.00	13.10	9.20	11.40
0.538	20	DES 1150	20.60	7.80	11.60	13.10
0.110	21	DES 1200	19.40	7.40	6.00	9.80
0.441	22	DES 1700	17.90	9.60	5.90	8.20
0.659	23	DESMOLAC 4200	18.70	9.60	9.90	8.20
0.148	24	M-NAL SM510N	19.90	8.10	6.00	9.80
0.429	25	SUP BECK 1001	23.26	6.55	8.35	19.85
0.815	26	PHENODUR 373U	19.74	11.62	14.59	12.69
1.130	27	P-LYTE S-100	16.47	0.37	2.84	8.59
1.176	28	PICCOPALE 110	17.55	1.19	3.60	6.55
0.254	29	P-RONE 450L	19.42	5.48	5.77	9.62
0.951	30	POLYSAR 5630	17.55	3.35	2.70	6.55
0.210	31	HYCAR 1052	18.62	8.78	4.17	9.62

DP = Dispersion Parameter
HP = Hydrogen-bond Parameter
PP = Polarity Parameter
R = Radius of sterical phase diagram

The properties and rankings for other agent contaminants and decontaminants are not available and should be determined.

3.3 Compatibility Rankings.

The compatibility approach to providing a candidate list exploits the compatibility charts that many material manufacturers provide for their materials against common industrial liquids. The compatibility charts are usually provided in terms of 3-10 rankings. The proposed strategy is to select a specific industrial liquid(s) on each chart for each chemical agent/decontaminant based on the ability of that liquid to predict agent interaction with the materials.

Examples of typical industrial compatibility charts are provided. One might select triethylphosphate[5] as the chemical representing GD (Table 9). In a few cases, an actual component of DS2[6] might have been tested (Table 10).

A few computerized chemical compatibility databases have been compiled. An example of the RAPRA Chemical Resistance database[7] contents is provided (Table 11).

3.4 Estimation Models.

Beyond DoD there is a widespread need for evaluating and ranking protective materials. The U.S. Environmental Protection Agency and U.S. Food and Drug Administration employ estimation methods that provide an initial screening or selection of materials based on interaction with chemicals. Investigators at MIT, A.D. Little, Incorporated[8,9] (Cambridge, MA), and other labs have modified estimation methods to accelerate the protective materials selection process.

One example of the output from the typical estimation technique is shown in Table 12. Several candidate protective materials are listed in the first column. "Experimental" versus "predicted" diffusion coefficients and solubilities are listed in the remaining columns. Low solubilities and low diffusion predict low permeation rates and more highly protective and resistant polymer for the specific liquid.

3.5 Accelerated CDMD Evaluation.

Another part of the material selection task would involve an acceleration of a systematic approach to enhance the CDMD. The current configuration of the CDMD is single-query oriented in which test results on either one material liquid pair or one material is retrieved.

Table 9. Example of Commercial Polymer Liquid Compatibility Data for Potential Database Use: Pyroite with Trialkyl Phosphates (Agent Simulants)[5]

CHEMICAL	PYROITE II 200°F	KYMAR 200°F	STAINLESS STEEL 316 70°F	TEFLON FEP 70°F	EPOXY 70°F	MASTELLOY C 70°F	VINYL ESTER THERMOSET 70°F	TEFLON PFA 200°F	PYROITE I 70°F
Tri Butyl Phosphate	A	A to 212°F	A to 70°F	A to 200°F	AB	--	AB to 140°F	A	AB to 150°F
Triethyl Phosphate	A	--	A	A to 200°F	--	--	AB to 100% to 200°F	A	A to 200°F

Table 10. Example of Commercial Polymer Liquid Compatibility Data for Potential Database Use: Plasite with Diethyl Triamine (DS2 Component)[6]

CHEMICAL EXPOSURE	TEMP °F	C-725	1244	3055	3066	6000	7100	7111	7122	7133	7155	7155 HHB	7156	9060	9080	9570
Diethylene Triamine	70°F			OK			F 5 3 Da	F 5 3 Da	F 5 3 Da	F 5 3 Da	F 5 3 Da					F 5 12 Da

Table 11. Example of Output of Chemical Resistance Database Developed by the Rubber and Polymer Research Association (RAPRA)

Chemicals and weightings:

1 Methyl ethyl ketone[9]
2 Acetone[8]
3 Acetophenone[8]
4 Cyclo-hexanone[8]

24 Polymers Selected for Current Short List

	Polymer (Code)	Rating	1	2	3	4
26	Polyphenylene sulphide (PPS)	297	S	S	S	S
9	Fluorinated ethylene propylene cop (FEP)	297	S	S	S	S
28	Polypropylene (PP)	297	S	S	S	S
13	Polyamide 6:10 (PA 6:10)	297	S	S	S	S
22	Polyimides (PI)	297	S	S	S	S
15	Polyamideimide (PAI)	297	S	S	S	S
14	Polyamide 6:6 (PA 6:6)	297	S	S	S	S
35	Perfluoroakloxyethylene (PFA)	297	S	S	S	S
42	Phenol-formaldehyde (PF)	297	S	S	S	S
30	Polytetrafluoroethylene (PTFE)	297	S	S	S	S
7	Ethylene-tetrafluorethylene (ETFE)	297	S	S	S	S
6	Ethylene-chlorotrifluorethylene (ECTFE)	281	S	S	P	S
39	Furane (F)	281	S	S	P	S
18	Polyether ether ketone (PEEK)	265	S	S	P	P
19	Polyethylene - High density (HDPE)	265	S	L	S	S
21	Polyethylene terephthalate (PET)	265	S	S	L	S
11	Polyamide 11 (PA 11)	265	S	S	S	L
12	Polyamide 12 (PA 12)	265	S	S	S	L
16	Polybutylene terephthalate (PBTP)	233	S	L	P	P
32	Polyvinylidene fluoride (PVDF)	229	L	L	S	S
4	Chlorinated polyethylene (CPE)	229	L	L	S	S
20	Polyethylene - Low density (LDPE)	229	L	S	L	S
24	Polymethylpentene (PMP)	217	S	L	S	D
34	Surlyn ionomer (EMA)	197	L	P	P	L

Table 12. Example of Estimation Approach: Comparison of Predicted Diffusion Coefficient and Solubility Values with Those Reported in Literature[9]

	Diffusion Coefficients (cm^2/s)		Solubilities (g/cm^3)		
	Experimental	Predicted	Experimental	Predicted UNIFAC	Predicted Kumar EOS
Natural Rubber					
Acetone	4.18E-07	3.39E-07	0.095	0.10	[illegible].006
Cyclohexane	3.4E-07	2.34E-07	2.8	4.1	0.25
Isopropanol	3.0E-08	3.28E-07	0.04	0.048	0.003
b-Propiolacetone	1.62E-07	2.74E-07	0.009	--	0.040
Toluene	4.48E-07	2.14E.07	3.5	3.7	0.59
Butyl Rubber					
Acetone	--	1.18E-07	0.037	0.028	0.026
Cyclohexane	1.61E-07	9.12E-08	2.2	3.6	0.048
Dimethylhydrazine	--	1.15E-07	0.09	--	0.028
Epichlorohydrin	--	8.53E-08	0.047	0.013	0.36
Ethylenimene	--	1.46E-07	0.13	0.26	0.036
Hexamethylphosphoramide	--	5.38E-08	0.07	--	0.95
Toluene	2.40E-07	8.57E-08	1.5	0.77	0.12

EOS = Equation of state
UNIFAC = Universal quasi-chemical functional group contribution activity coefficient equation

The enhancements would exploit the capabilities inherent in a relational database. A systematic sequence can be listed and included (see Table 13):

Table 13. Systematic Strategy for a Materials Science Approach to Enhancing the Capabilities of a Materials Database

- Programmed Self-Inventory
  Occurrence/Nonoccurrence of Data and Ratings

- Programmed Self-Critique
  Deviation from Standards
  Material Specimen Documentation
  Test Versus Property Identifier
  Disclaimers, Warnings

- Programmed Self-Evaluation
  Define Equivalence/Nonequivalence
  Trends

- New Search Strategies
  Material Selection
  Material Ranking
  Material Benchmark Sorting
  Agent Decontaminability and Decontaminability Hardness

- Revised Report Forms

A long-term enhancement would be a technical base task for the CRDEC Data Management Office. The accelerated task would attempt to rapidly derive candidate-recommended materials from the CDMD before and during long-term revisions.

3.6 Strategy for Generation and Update of a Materials Guide.

Recommended strategy to maximize the capability of a CDMD for the generation of ranked and recommended candidate materials is the systematic development of standard material test methods and data generation based on these methods. This strategy can be accelerated by the methods discussed herein and summarized in Table 14. The estimation methods (Section 3.4) are not included, because the method performance has not been established. The systematic and accelerated strategies can be developed in parallel and coordination maintained by defining each of the material rankings from Table 13 as a small "test" in the CDMD.

Table 14. Candidate NBCCS Survivable Materials Guide[7]

Rank and Recommendation Based on:

- Commercial polymer liquid interaction databases validated by ASTM D3132 Test

- Commercial compatibility compilations and databases by selecting solvent entries closest to agents and decontaminants for each

- Accelerated systematic evaluation of Chemical Defense materials database providing an Interim Updated Material Guide

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4. CONCLUSIONS AND RECOMMENDATIONS

A limited but potentially useful NBC Contaminated Survivable (NBCCS) materials guide is feasible. An NBCCS guide would be limited by the following constraints:

- The guide would have to be subdivided into numerous "application critical" material lists. The guide would probably be more accurate at excluding a large portion of material candidates for an application as opposed to recommending a select group of candidates.

- The guide would only generate a reduced list of "candidates." The responsibility of ensuring the NBC contamination survivability of the final material selection would remain with the system developer. Test methodology and associated chemical surety materials contractor testing programs are being developed to help Department of Defense system developers in fulfilling their NBCCS responsibilities in the final testing and selection of materials.

The systematic development of the materials evaluation capabilities of the Chemical Defense Materials Database should continue. The integration of accelerated materials evaluation capabilities is feasible and can be accomplished as resources become available.

LITERATURE CITED

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APPENDIX A

CHEMICAL BIOLOGICAL INFORMATION AND ANALYSIS CENTER'S (CBIAC) ROLE IN NBC CONTAMINATION SURVIVABILITY (NBCCS)

James J. McNeely

CBIAC continues to be inundated with inquiries related to the NBCCS of materials and systems.

Heightened interest in this area has been generated by recently established instructions and regulations that mandate that all new materiel be developed to be survivable in NBC contaminated environments. Specifically, DoD Instruction (DoDI) 4245.13, dated 15 June 1987, states that "NBCCS will be included in the design of systems that must perform mission-essential functions in an NBC environment." An NBCCS system defined as one that is hardened against NBC contamination and decontaminants, can be decontaminated, and is compatible with individual protective equipment. In compliance with DoDI 4245.3, the U.S. Army, U.S. Navy, and U.S. Air Force have taken action and prepared documents for implementing this DoDI. The implementing documents are Army Regulation 70-71 (which preceded the DoDI), NAVSEC Instruction 3400.2, and U.S. Air Force Regulation 80-38 (revised version).

Unfortunately, within the scope of our inquiry service, the CBIAC cannot provide a definite answer when asked if a system or material is NBCCS. The reason for this is that very few, if any, materials or systems have been tested in a manner that provides a definite answer to the question. Part of the problem is that many survivability criteria are stated in operational terms that are difficult to quantify. Operational testing needed to provide unambiguous answers is often either cost-prohibitive or simply not feasible. As a result, developers are forced to draw inferences on NBCCS using preliminary data normally used only for screening purposes. To complicate the issue, standardized test methods have not been used to generate the preliminary data. As a result, it is often difficult to make even relative comparisons of the resistances of materials to NBC contaminants and associated decontaminants.

Despite the problems identified above, CBIAC attempts to provide as much assistance as possible to developers faced with meeting NBC survivability requirements. This assistance is provided through our inquiry and special study services. In our inquiry service, CBIAC staff provides assistance by identifying and retrieving relevant test data for developers upon request. To provide this information, the staff accesses information resources that provide most of the materials' compatibility data currently available, which include the U.S. Air Force Materials Compatibility Database and the databases at the Defense Technical Information Center. In addition, the U.S. Army's NBCCS office has provided CBIAC with invaluable assistance and guidance in understanding the problem and identifying potential solutions.

Through the special studies function, more detailed survivability assessments of materials and systems are performed. In performing these assessments, researchers apply a methodology developed for the U.S. Army's NBCCS office. The goal of these assessments is to identify potential problems and recommend solutions. Often, critical data gaps are identified, and test plans for filling critical data gaps are developed.

APPENDIX B

ASSESSMENT OF THE STATUS OF THE NBC CONTAMINATION SURVIVABILITY (NBCCS) MATERIALS DATABASE

James J. McNeely

Determining whether or not materials and/or systems satisfy NBCCS requirements is a problem for two reasons. First, very few, if any, materials or systems have ever been tested against the full-range of agents and decontaminants of concern. Second, test methods that have been used to collect existing compatibility data do not provide answers to the questions raised by new survivability requirements (e.g., those outlined in Army Regulation 70-71).

A recent survey of the U.S. Air Force Materials Compatibility Data-base demonstrates just how severe the current data gaps are. The U.S. Air Force database is the most comprehensive collection of compatibility data available. This database contains test results compiled from 56 test programs and data for 655 specific materials that can be categorized into 184 generic material types. None of the 655 specific materials has been tested against the full-range of agents (GD or TGD, HD or THD, VX) and decontaminants (DS2 and STB) of concern. Only six (Table B-1) of the 184 generic types have been tested for any of the test properties. For purposes of this discussion, we will call these materials Class I materials for any "mix" or "match" of the test properties.

Table B-1. Generic Materials Tested Against GD or TGD, HD or THD, VX, DS2, and STB

Code	Polymeric material	Classification
PC	Polycarbonate	Plastics
PE	Polyethylene	Plastics
PMMA	Poly(methylmethacrylate)	Plastics
PTFE	Polytetrafluoroethylene	Plastics
PUR	Polyurethane	Plastics
PUR/PARA	Polyurethane/Polyarylamide	Plastics

Even after relaxing the requirements, significant gaps remain. Only 31 (Table B-2) of the 184 generic material types have been tested against any of the nerve agents (GD, TGD, VX), mustard (HD and THD), and

two decontaminants (DS2 and STB). For purposes of this discussion, we will call these materials Class II materials.

Table B-2. Generic Materials Tested Against GD or TGD or VX, HD or THD, DS2, and STB

Code	Material	Classification
A92024	Wrought Aluminum Alloy 2024	Metals
A96061	Wrought Aluminum Alloy 6061	Metals
A97075	Wrought Aluminum Alloy 7075 Material	Metals
BIIR	Bromo-Isobutene-Isoprene	Elastomers
CA	Cellulose Acetate	Plastics
CO	Polychloromethyl Oxirane	Elastomers
CR	Chloroprene	Elastomers
EP	Epoxy, Epoxide	Plastics
FKM	Fluoro Rubber - Polymethylene Type	Elastomers
FVMQ	Silicone Rubber/Fluorine	Elastomers
M11311	Wrought Magnesium Alloy, Extruded AZ31	Metals
MQ	Silicone Rubbers/Methyl Group	Elastomers
NBR	Acrylonitrile-Butadiene (Buna N)	Elastomers
NR	Natural Rubber	Elastomers
OT	Rubber with C, S, and O in the Chain	Elastomers
PARA	Polyaryl Amide	Plastics

Table B-2. Generic Materials Tested Against GD or TGD or VX, HD or THD, DS2, and STB (Continued)

Code	Material	Classification
PC	Polycarbonate	Plastics
PE	Polyethylene	Plastics
PET	Poly(ethyleneterephthalate)	Plastics
PMMA	Poly(methylmethacrylate)	Plastics
POP	Poly(phenyleneoxide)	Plastics
PPSU	Poly(phenylenesulfone)	Plastics
PTFE	Polytetrafluoroethylene	Plastics
PUR	Polyurethane	Plastics
PUR/PARA	Polyurethane/Polyaryl Amide	Plastics
PVC	Poly(vinyl chloride)	Plastics
PVC/PET	Poly(vinyl chloride)/ Poly(ethylene terephthalate)	Plastics
PXY	Parazylene	Plastics
SBR	Stryene-Butadiene (Bune S) (Gr-S)	Elastomers
TYPES	Thermoplastic Polyester (Gereral)	Plastics

Property ratings for Classes I and II materials are provided in Table B-3. These ratings indicate the effects of a particular chemical (GD or TGD, HD or THD, VX) and decontaminants (DS2 and STB) upon a particular property of a material. For the most part, the ratings have been assigned as follows:

Negligible: If property change >= 0 and <= 5

Moderate: If property change > 5 and <= 10

Major: If property change > 10 and <= 25

Severe: If property change > 25

A tally of the occurrences of property data is provided in Table B-4.

Property ratings for Classes I and II materials for the range of agents and decontaminants for the property "weight" are provided in Table B-5.

Table B-3. Property Ratings for Classes I and II Materials

Material Code	Major	Moderate	Negligible	Severe	Total
PC	15	14	31	48	108
PE	16	13	44	7	80
PUMMA	44	42	90	63	239
PTFE	17	16	29	2	64
PUR	12	6	23	20	61
PUR/PARA	2	1	0	2	5
A92024	10	0	15	2	27
A96061	0	0	4	0	4
A97057	0	0	4	0	4
BIIR	4	7	38	1	50
CA	5	3	16	21	45
CO	12	15	29	10	66
CR	8	8	17	1	34
EP	24	22	27	13	86
FKM	15	7	37	5	64
FVMQ	9	8	26	13	56
IIR	14	15	85	2	116
M11311	0	0	4	0	4
MW	34	21	59	30	144
MBR	15	10	21	140	56
NR	16	15	39	5	75
OT	15	16	29	6	66
PARA	4	2	5	36	47
PET	3	1	13	3	20
POP	9	11	35	10	65
PPSU	11	9	29	17	66
PVC	6	7	41	24	78
PVC/PET	3	0	2	1	6
PXY	0	1	3	0	4
SBR	9	14	38	2	63
TPES	1	2	6	1	10

Table B-4. Tally of the Occurrences of Property Data (for all Materials in the Database)

Property Code	Number of Occurrences
ASBRP.RATE	27
ASBRP.RTE	1
ADH.STR	2
AREA	15
BARCOL.HRD	43
BD.SRF.DUR	12
BKR.CPCTY	1
BRK.CPCTY	68
BRK.TIME	108
BURST.STR	2
CHM.PUR.D	2
CHM.PUR.DG	9
CMPRSN.SET	20
CMPRSV.STR	2
CORR.RATE	294
CUM.EVAP	10
CUM.PENT	231
DIAM	28
DIELE.STR	14
DIFFUSIV	54
DSRP.RATE	26
ELO.YLD	53
FLEX.MD	4
GL.TRN.TMP	35
HAZE	18
HT.DFL.TMP	35
IM.STR.IZN	15
LENGTH	32
LOAD.DEF1	2
LOAD.DEF5	2
MAX.ELO	423
MD.ELA.T	172
MP	13
PERM.RATE	48
PIT.DEPTH	4
PL.STR.AVG	40
RED.AREA	28
ROCK.HRD	36
SHOR.A.HRD	213
SHOR.A.HRD	60
SOLUBLTY	4
TEAR.RSTN	20

Table B-4. Tally of the Occurrences of Property Data (for all Materials in the Database) (Continued)

Property Code	Number of Occurrences
TGH.AREA	24
TGH.DMNLSS	80
THCK.CNTR	175
THCK.EDGE	8
TN.STR.100	140
TN.STR.300	19
TN.STR.BRK	594
TR-10.RTRC	20
TRNSM.0.4	6
TRNSM.0.5	6
TRNSM.0.6	6
TRNSM.0.7	6
TRNSM.ACT	18
VOL.SWELL	45
WEIGHT	622
WIDTH	32
YLD.STR	107

Table B-5. Tally of the Ratings of the Property Weight

Material Code	Major	Moderate	Negligible	Severe	Total
A92024	0	0	4	0	4
BIIR	0	0	4	0	4
CA	0	1	1	8	10
CO	0	1	3	0	4
EP	1	1	4	0	6
IIR	0	0	8	0	8
MQ	2	1	4	1	8
NR	0	4	3	0	7
PC	0	0	0	6	6
PE	0	0	7	0	7
PET	0	0	1	3	4
PMMA	2	1	6	1	10
POP	0	0	4	0	4
PPSU	0	0	3	1	4
PTFE	0	0	2	0	2
PUR	1	0	4	1	6
PVC	1	0	4	6	10
PXY	0	1	1	0	2
SBR	2	3	12	0	17

APPENDIX C

METHODS FOR GENERATING FUNDAMENTAL MATERIALS COMPATIBILITY DATA

C-1. INTRODUCTION

The following discussion identifies an approach that may be employed to generate fundamental materials compatibility data.

The tests identified and recommended are grouped into three tiers. The number, complexity, and expense of the tests increase as one proceeds from the first to the third tier. The objective of the approach outlined here is to optimize the return on investment. This can be accomplished using the simple and inexpensive tests identified in the lower tiers as a means to screen and limit the number of materials requiring subsequent testing that is more complex and expensive.

C-2. BASIC EXPOSURE TESTING

The simplest, most-basic, and least-expensive approach to screening for the degree of compatibility or interaction between liquids and polymeric materials is the solubility determination on uncrosslinked polymer. A standardized solution test is American Society for Testing and Materials (ASTM) D-3132. This test is not yet exploited in the Chemical Defense Material Database. Therefore, the first step in determining the compatibility of a particular material should involve generating basic exposure data. The universally accepted means of generating such data is to determine the weight change (loss or gain) of a material when it is exposed to a chemical. Review of the tally of property data in the current database (Table C-1) supports this claim. More data exist for weight change than for any other property. This is even more apparent if one considers that many other properties (e.g., corrosion rate) are actually calculated from weight-loss data.

Fortunately, weight change is not only a good indicator of the resistance of materials to chemicals (hardness). Weight change is also a good indicator of the potential NBC contamination survivability (NBCCS) hardness and decontaminability of materials. This is especially true if the tests are conducted in such a fashion that desorption (off-gassing) is monitored either during or after the test. More work is needed to define methods for generating desorption data.

The ASTM specifications for determining the resistance of major classes of materials to chemical reagents are listed in Table C-2. All but one of these specifications (adhesive resistance) describes methods for performing weight-change tests. The specifications also describe methods for collecting additional information (e.g., changes in appearance, dimension, and volume) that is useful in characterizing the chemical resistance of a material. Finally, the specifications listed (Table C-3) reference additional tests (and associated specifications) that should be performed

to determine the chemical resistance of materials. Most of the additional tests are mechanical property tests.

Table C-1. Tally of Properties Tested in Current Database

Property	Number of Occurrences
Abrasion Resistance	1
Absorption Rate	27
Adhesive Strength	2
Appearance	1
ARC Resistance	1
Barcol Hardness	43
Bearing Strength	1
Bearing Yield Strength	1
Bond Surface Durability	12
Breaking Load	1
Breakthrough Time	108
Brinell Hardness	1
Bulk Modulus of Elasticity	1
Burst Strength	2
Chemical Purity Degradation	9
Color	1
Compression Set	20
Compressive Strength	2
Corrosion Rate	294
Creep Rupture Strength	1
Creep Strength	1
Cumulative Penetration	231
Desorption Rate	26
Diameter	28
Dielectric Constant	1
Dielectric Strength	14
Diffusivity	54
Dissipation Factor	1
Elastic Limit	1
Elongation (Yield)	53
Fatigue Strength	1
Film Hardness	1
Flexural Modulus	4
Flexural Strength	10
Flexural Stress	1
Glass Transition Temp. (TG)	35
Haze	18
Heat Deflection Temperature	21
Impact Strength (CHARPY)	1
Impact Strength (IZOD Notched)	15
Impact Strength (IZOD-Unnotch)	1

Table C-1. Tally of Properties Tested in Current Database (Continued)

Property	Number of Occurrences
Index of Refraction	1
Integrity	1
Knoop Hardness	1
Length	32
Load Deformation (1st Cycle)	2
Load Deformation (5th Cycle)	2
Maximum Elongation	423
Melting Point	13
Mod. Elasticity (Shear/Torsion)	1
Mod. Elasticity (Tension/Comp.)	1
Modulus Elasticity (Tensile)	172
Modulus of Resilience	1
Modulus of Rupture in Bending	1
Modulus of Rupture in Torsion	1
Optical Abrasion Resistance	1
Peel Strength (Average)	40
Penetration Rate	1
Permeability	1
Permeation Rate	48
Pitting Depth	4
Poisson's Ratio	1
Power Factor (100,10E3,10E6 HZ)	1
Reduction of Area	28
Rockwell Hardness	36
Shear Strength	1
Shore A Hardness	213
Shore D Hardness	60
Slit Propagation	12
Solubility	4
Solubility at Infinite Dilut.	1
Stiffness	1
Stress Craze	1
Surface Area	15
Surface Resistivity	1
Tear Resistance	20
Tearing Strength	1
Tensile Strength (100% Elong.)	140
Tensile Strength (300% Elong.)	19
Tensile Strength (Break)	594
Tensile Strength (Yield)	107
Thickness(Center)	175
Thickness (Edge)	8
Toughness (Area)	24
Toughness (Dimensionless)	80
TR-10 Retraction	20

Table C-1. Tally of Properties Tested in Current Database (Continued)

Property	Number of Occurrence
Transmittance (0.4u)	6
Transmittance (0.5u)	6
Transmittance (0.6 μ)	6
Transmittance (0.7 μ)	6
Transmittance (Actual)	18
Vickers Hardness	1
Volume (Swell %)	45
Volume Resistivity	1
Weight	622
Wettability	1
Width	32
Yield Point	1
	82

Table C-2. ASTM Specifications for Chemical Resistance

Material Class	Specification
Metals	ASTM G-31
Plastics	ASTM D-543
Composites	ASTM D-543
Elastomers	ASTM D-471
Adhesives	ASTM D-896

C-3. MECHANICAL PROPERTY TESTING

Once basic exposure data have been generated, tests should be performed to generate data on the effects of agents and decontaminants upon the functional properties of materials. These data are intended to indicate whether materials will perform their intended function after contamination and/or decontamination. Materials that performed poorly in the basic exposure tests may be eliminated from consideration for functional property testing.

Functional properties of materials are typically divided into the following basic categories:

- Mechanical
- Optical
- Electrical
- Thermal
- Adhesive
- Barrier

Table C-3. Tally of Test Specifications in Current Database

Test Specification	Number of Occurrences
ASTM	1
ASTM 543-67	2
ASTM 740-63	1
ASTM C-794	20
ASTM D 1876-72	4
ASTM D 2240-77	1
ASTM D 543-67	1
ASTM D 740-63	4
ASTM D-1003	32
ASTM D-1329-60	20
ASTM D-2240	169
ASTM D-2583	4
ASTM D-3762	12
ASTM D-380	2
ASTM D-395	21
ASTM D-412	538
ASTM D-471	334
ASTM D-471-77	1
ASTM D-622	3
ASTM D-624	20
ASTM D-638	368
ASTM D-741	1
ASTM D-790	8
ASTM D1876-72	16
ASTM D2240-77	73
ASTM D412	5
ASTM D412-75	96
ASTM D412-77	2
ASTM D471-77	125
ASTM D543-67	83

Table C-3. Tally of Test Specifications in Current Database (Continued)

Test Specification	Number of Occurrences
ASTM D622	1
ASTM D638	1
ASTM D638-77	132
ASTM D740-63	1
ASTM E-8	165
CWS DIRECTIVE 210	13
NA	32
NS	1692
PARA 4.5.6 MIL-C-25769H	1
PARA 4.5.7 OF MIL-C-24769H	1
PARA 4.5.7 OF MIL-C-25769H	94
PARA 4.5.7 OF MIL-S-25769H	1
PARA. 4.5.7 OF MIL-C-25769H	3
THERMAL MECHANICAL ANALYZER	25
THERMAL MECHANICAL ANALYZES	1

Mechanical properties are usually tested while determining the chemical resistance of materials. This may be true for two reasons. First, most materials (particularly metals, plastics, elastomers, and composites) are most often used in applications in which only mechanical properties are critical. Second, mechanical properties tend to be critical even if other properties are only of interest. A good example of such a case is the selection of a material to be used in an aircraft canopy. In this case, the optical and mechanical properties of the material are critical to the performance of the item.

Specifications for generating basic mechanical properties data are provided in Table C-4. These specifications are cross-referenced by the ASTM specifications for chemical resistance listed in Table C-2. Because there may be several mechanical properties identified within each specification, some control must be imposed to limit the number of properties actually tested. The mechanical properties most commonly tested in chemical resistance testing are tensile strength (at break), maximum elongation, and modulus of elasticity. Again, the tally of the data in the current database indicates that this has also been the case for CW compatibility testing.

Table C-4. Specifications for Mechanical Property Testing Tensile

Material Class	Specification
Metals	ASTM E-8
Plastics (0.4 --> 0.55-in. thick)	ASTM D-638
(<0.04-in. thick, films)	ASTM D-882
Elastomers	ASTM D-412
Composites	ASTM D-638 ASTM D-3039 (laminates)
Adhesives	ASTM D-897 ASTM D-2095*

*ASTM D-2095 supersedes ASTM D-897

Material hardness deflection (not NBCCS "hardness") data has also been generated quite often in past compatibility programs. For the sake of completeness, specifications for hardness tests are provided in Tables C-5 and C-6.

Please note that although mechanical tests for adhesives do exist (ASTM D-897 and D-2095), these tests have not been used in past CW compatibility testing. In some cases, tests methods for determining the mechanical properties of elastomers (ASTM D-412) have been substituted for the analogous test methods for adhesives. In other cases, tests of shear and peel strengths have been used for tensile strength tests. The justification for making these substitutions should be confirmed.

Table C-5. Specifications for Mechanical Property Testing Hardness

Material Class	Property	Specification
Metals		ASTM E-18
		ASTM D-3648
Plastics	Shore A, D	ASTM D-3648
	Rockwell	ASTM D-785
	Barcol	ASTM D-2583
	Shore A, D	ASTM D-2240
Elastomers	Shore A, D	ASTM D-2240
	Vicat Softening	ASTM D-1525
	Shore A	ASTM D-3242
Adhesives	Shore A, D	ASTM D-2240
	Shore A	ASTM D-3242

Table C-6. Specifications for Mechanical Property Testing Deflection/Expansion

Material Class	Property	Specification
Plastics	Heat Deflection Temperature	ASTM E-18
	Glass Transition Temperature	ASTM TM01-01A
	Melting Point	ASTM D-2117
	Linear Thermal Expansion	ASTM E-2117
	Coefficient of Linear Expansion Electrical	ASTM D-3386

C-4. SPECIFIC FUNCTIONAL PROPERTY TESTING

Once basic exposure mechanical data have been generated, additional testing may be performed to determine if properties critical to the specific function of the material are degraded by chemical exposure. Classic examples of such properties are transmittance for optical materials and resistivity or dielectric strength for electrical materials. Again, if a material performed very poorly in basic exposure or mechanical property tests, the material should not even be considered for functional property testing.

Examples of specifications for generating functional property data are provided in Table C-7.

Table C-7. Examples of Specifications for Functional Property Testing

Property Class	Material Class	Property	Specification
Optical	Plastics	Transmittance	ASTM D-1003
Electrical	Plastics	Dielectric Strength	ASTM D-149,D-150
		Resistivity	ASTM D-257
	Elastomers	Resistivity	ASTM D-991
Adhesive	Adhesives	Shear Strength	ASTM D-1002
		Peel Strength	ASTM D-1876

C-5. TEST CONDITIONS

Although ASTM specifications listed in Table C-2 recommend specific test conditions for determining chemical resistance, some of these test conditions must be modified for CW compatibility testing. Specifically, exposure concentrations (contamination densities) and times recommended by ASTM must be redefined because they are too severe for CW compatibility testing. For example, ASTM specifications call for materials samples to be completely immersed in chemical reagents from days (for polymers) to months (metals).

In some of the more recent and rigorous CW compatibility test programs, the following standards seem to have been established.

- Exposure Temperatures:

  23 and 71 °C

- Exposure Concentrations:

  Decontaminants: Total Immersion

  Contaminants: Droplets at 8 and 80 g/m^2

- Exposure Periods:

  0.5, 1, 4 or 6, and 24 hr

Some questions still remain as to whether or not the agent contamination densities listed above are sufficient for generating reproducible data. The concern is that small quantities may not cover samples uniformly or that the quantity of agent may not remain constant throughout the test for volatile reagents. This issue should be addressed before additional testing is initiated.